Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models

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Supporting Information

Supplementary Material

Comparison of Thermodynamic Properties

of Coarse-Grained and Atomic-Level Simulation Models

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Supplementary Tables

TABLE s 1: Hydration free energies of aliphatic hydrocarbons in water from experiments (ΔF_{hyd}^{exp}) and from MD simulation at different model resolutions (ΔF_{hyd}^{CG} and ΔF_{hyd}^{AL}), as displayed in Figure 2. Values from thermodynamic integration (and corresponding errors) are displayed for CG (r_1 = 0.0 nm; r_c = 1.4 nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in kJ mol^{-1}.

TABLE s 2: Solute-solvent interaction energy change upon hydration (ΔU_{uv}) for C4, C8, C12 and C16 in water, as displayed in Figure 3. Values from thermodynamic integration (and corresponding errors) are displayed for CG (r_1 = 0.0 nm; r_c = 1.4 nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in kJ mol^{-1}.

TABLE s 3: Solvent-solute entropy change upon hydration (ΔS_{uv}) for C4, C8, C12 and C16 in water, as displayed in Figure 4. Values from thermodynamic integration (and corresponding errors) are displayed for CG CG (r_1 = 0.0 nm; r_c = 1.4 nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in J mol^{-1} K^{-1}.

TABLE s 1:

	$\Delta F_{hyd}^{exp,\,a}$	ΔF_{hyd}^{CG} and $\Delta F_{hyd}^{AL,b}$									
	298 K	263 K		283 K		303 K		323 K		343 K	
		CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
n-butane	9.0	10.1 (0.3)	6.4 (0.9)	11.9 (0.3)	8.5 (0.8)	13.7 (0.3)	9.6 (0.8)	15.3 (0.3)	10.0 (0.9)	16.9 (0.3)	10.9 (0.9)
n-octane	12.1	13.6 (0.4)	6.6 (1.7)	16.5 (0.4)	9.0 (1.5)	19.8 (0.4)	11.9 (1.5)	22.8 (0.5)	12.1 (1.7)	25.5 (0.5)	14.3 (1.8)
n-dodecane	---	19.3 (0.6)	8.5 (1.7)	24.8 (0.5)	12.0 (1.7)	29.4 (0.5)	17.9 (1.7)	34.1 (0.5)	18.3 (1.7)	38.5 (0.6)	21.0 (1.8)
n-hexadecane	---	24.7 (0.6)	10.9 (2.4)	30.5 (0.6)	14.7 (2.3)	36.9 (0.5)	19.7 (2.0)	43.5 (0.6)	21.6 (2.0)	48.2 (0.6)	25.9 (1.8)

[a] Experimental values taken from Ben-Naim and Marcus 1987.

[b] Calculated values are for N,V,T ensembles as described in the Computational Methods section. Volumes were different for each system and each temperature as obtained after equilibration at constant pressure.

TABLE s 2:

	ΔU_{uv}^{CG} and ΔU_{uv}^{AL}									
	263 K		283 K		303 K		323 K		343 K	
	CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
n-butane	-15.7 (0.3)	-38.6 (3.9)	-15.4 (0.3)	-37.7 (4.0)	-15.0 (0.4)	-35.6 (4.3)	-14.6 (0.4)	-35.2 (4.4)	-14.2 (0.4)	-33.5 (4.6)
n-octane	-29.5 (0.4)	-68.2 (5.1)	-29.0 (0.4)	-65.6 (5.2)	-28.6 (0.4)	-63.9 (5.4)	-28.0 (0.5)	-61.7 (5.6)	-27.4 (0.5)	-58.8 (6.0)
n-dodecane	-43.2 (0.5)	-97.1 (6.0)	-42.7 (0.5)	-94.4 (6.7)	-42.1 (0.5)	-90.4 (7.0)	-41.4 (0.5)	-87.1 (6.8)	-40.7 (0.6)	-84.3 (7.2)
n-hexadecane	-56.9 (0.5)	-126.8 (6.9)	-56.2 (0.6)	-122.6 (7.4)	-55.6 (0.6)	-115.0 (7.8)	-54.9 (0.6)	-112.2 (7.9)	-54.1 (0.7)	-108.1 (8.4)

TABLE s 3:

	ΔS_{uv}^{CG} and ΔS_{uv}^{AL}									
	263 K		283 K		303 K		323 K		343 K	
	CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
n-butane	-98 (1)	-171 (18)	-96 (1)	-163 (18)	-95 (1)	-149 (17)	-92 (1)	-140 (16)	-91 (1)	-129 (16)
n-octane	- 164 (1)	-284 (26)	-161 (1)	-264 (24)	-160 (1)	-250 (23)	-157 (1)	-228 (23)	-154 (1)	-213 (23)
n-dodecane	-238 (1)	-401 (29)	-238 (1)	-376 (30)	-236 (1)	-357 (29)	-234 (1)	-326 (26)	-231 (1)	-307 (26)
n-hexadecane	-310 (1)	-523 (35)	-306 (1)	-485 (34)	-305 (1)	-444 (32)	-305 (1)	-414 (30)	-298 (1)	-391 (30)

Supplementary Figures

Figure s 1: Free energy derivative of removing C4 from water for (a) CG or (b) AL simulations. $\langle \partial H/\partial \lambda \rangle$ values and their errors are shown from simulations at 263 K (cyan), 283 K (green), 303 K (black), 323 K (orange), and 343 K (red). The error bars have been estimated from block averaging. Simulation times per λ-point ranged from 3 to 15 ns (CG) or from 0.2 to 6 ns (AL).

Figure s 2: Solvent-solvent (reorganization) entropy change upon hydration (ΔS_{vv}) as a function of the simulation reference temperature for CG (empty circles) and AL (filled circles) simulations of (a) C4, (b) C8, (c) C12 and (d) C16.

Figure s 3: Lennard-Jones potential energy functions as defined and implemented in GROMOS05[51] (black line) and as defined (but not implemented) in the GROMACS manuals[50] (dashed line). The energy is displayed in the sample case of the interaction between two CG water beads as a function of their distance.

Figure s 1:

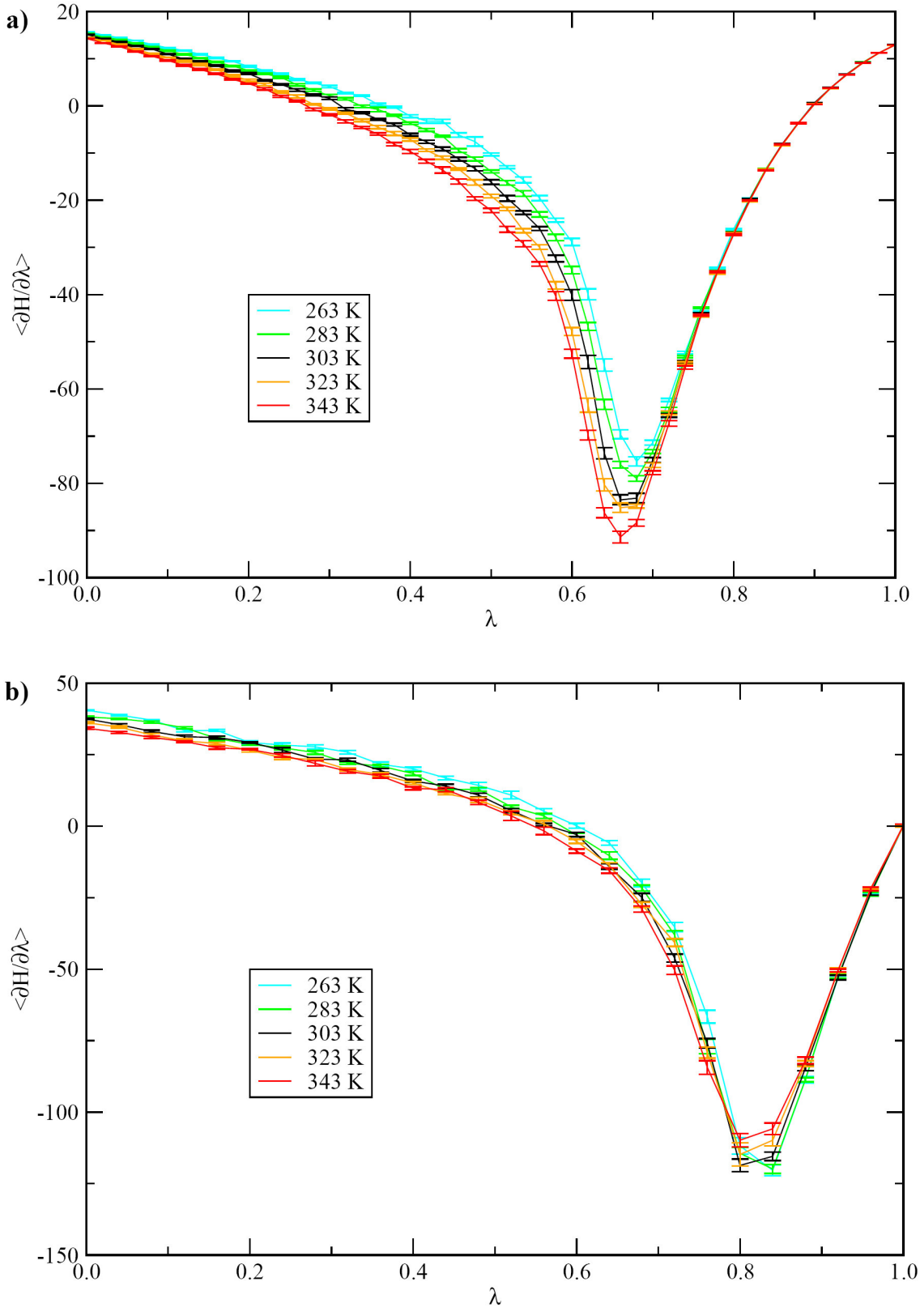

a)
20
0
-20
-40
-60
-80
-100
0.0
0.2
0.4
0.6
0.8
1.0
λ
<∂H/∂λ>
263 K
283 K
303 K
323 K
343 K
b)
50
0
-50
-100
-150
0.0
0.2
0.4
0.6
0.8
1.0
λ
<∂H/∂λ>
263 K
283 K
303 K
323 K
343 K

Figure s 2:

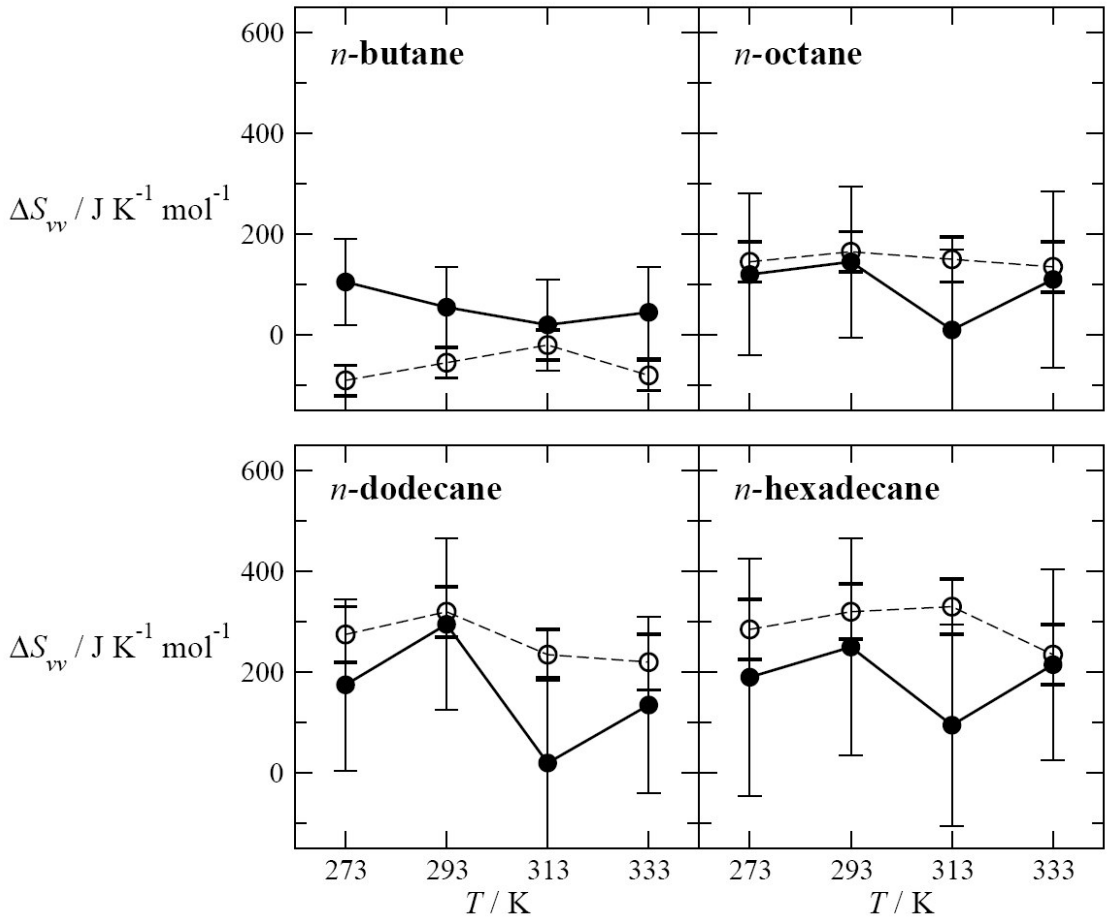
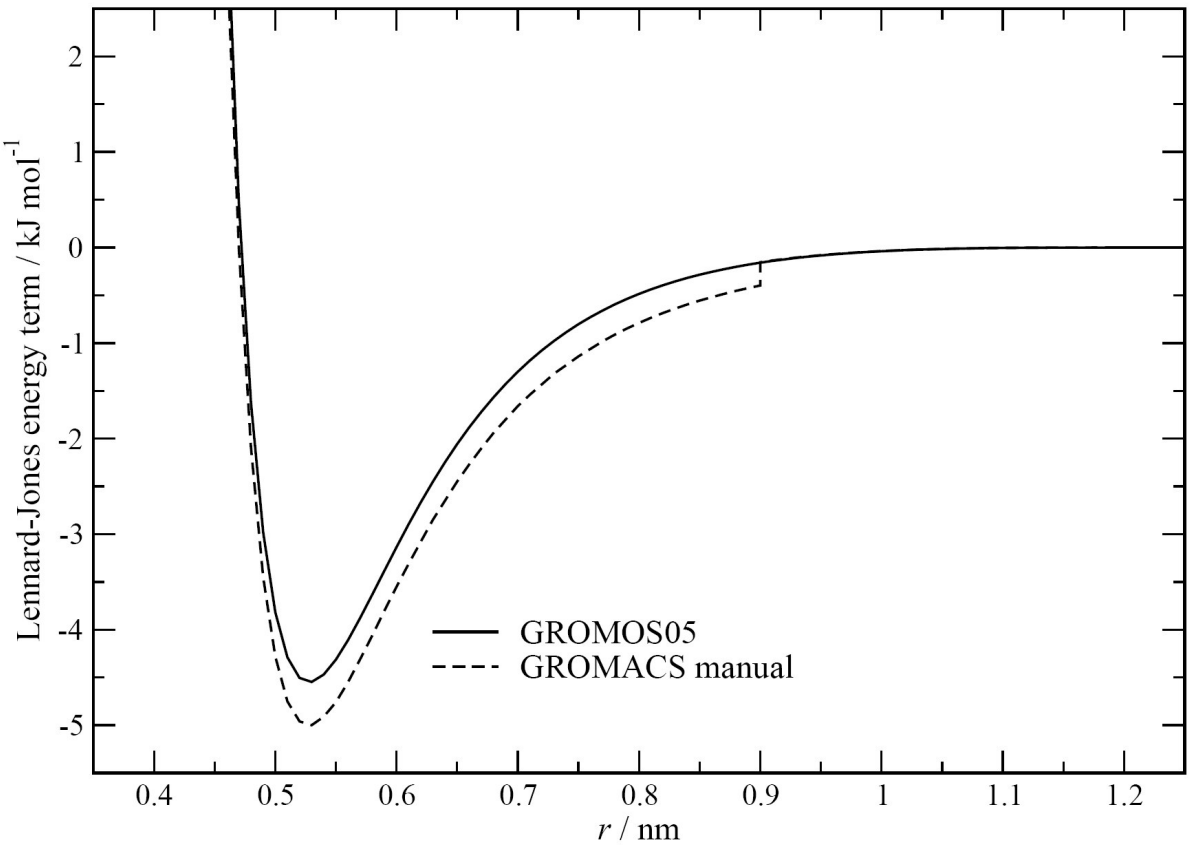

n-butane
n-octane
n-dodecane
n-hexadecane
ΔSvv / J K-1 mol-1
ΔSvv / J K-1 mol-1
600
400
200
0
273
293
313
333
T / K
T / K

Figure s 3:


Lennard-Jones energy term / kJ mol^{-1}
2
1
0
-1
-2
-3
-4
-5
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
r / nm
GROMOS05
GROMACS manual